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LABORATORY OF HIGH PRESSURE CHEMISTRY

Head: Dr. Yoshimasa Takezaki

This laboratory started in 1957 as a new section separated from Kodama Laboratory (Head: Prof. Dr. Shinjiro Kodama). The laboratory has been investigating high pressure organic synthetic chemistry, and on the other hand, though does not appear in the title, kinetical and mechanistic research on the free radical and atom reactions in gas phase as a main theme, too.

1. High Pressure Chemistry

As to the high pressure chemistry, effort has been devoted mainly to the gas and liquid (solid) reactions, to synthesize useful products such as aromatic aldehydes, carbonic mono- or dibasic saturated or unsaturated acids *etc.*, using carbon monoxide, carbon dioxide or hydrogen under the pressure of some hundred atmospheres as a reactant, and as substrates aromatic hydrocarbons, olifins, halo-benzenes, phenols, stylene, cyclohexene, alcohols allylic compounds, or aqueous alkali and even the solid material such as alkali acetate are used and the catalyst used are HF-BF_3, H_2SO_4, H_3PO_4, alkali carbonates, and $PdCl_2$ (and its complex).

The character of researches is mainly fundamental, *i.e.*, the reaction rate (and equilibrium) is being analyzed to establish the reaction mechanism, the results of which will be seen in the publication list at the end of this section.

2. Free Radical Chemistry

In this part, investigation on the rate constant determination and on the detailed mechanism of the elementary reactions involving free radicals and atoms in gas phase which are produced by various methods *e.g.*, (vacuum) ultraviolet photolysis, microwave discharge and combination of radicals and/or atoms produced by the above-mentioned processes for the production of unsaturated radicals. The technics utilized here are, a dynamical Time-of-Flight mass spectrometry and spectrometrical measurement for transients and the usual G-C analysis for stable products.

The character of the research is also kinetical, and the detailed mechanism of the unimolecular decomposition or isomerisation of chemically activated species such as methyl allyl ether, pentyl, 1-butene-1 or -4 yl radical has been elucidated with the aid of RRKM theory, further, on some reactions of O, Cl, NO_2, NO, N researches are now going on.

On the other hand, computational simulation of the process of photochemical air pollution utilizing the known rate data of some 100 elementary reactions is now in progress.

Publications

(* indicates an article published in Japanese)

I High Pressure Chemistry

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8. K. Kudo, N. Sugita, and Y. Takezaki: Kinetic Study of Potassium Molonate Synthesis from Potassium Acetate, Carbonate, and Carbon Monoxide under Pressure, *Nippon Kagaku Kaishi*, 1082 (1973).
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12. A. Yanagase, N. Sugita, K. Kudo, and Y. Takezaki: Kinetic Study on the Synthesis of Methyl Glycolate from Methylene Sulfate and Carbon Monoxide under Pressure, *ibid.*, 583 (1975).
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14. H. Yoshida, N. Sugita, K. Kudo, and Y. Takezaki: Kinetics on the Carbonylation of Cyclohexene in a Methanol Solution Catalyzed by Palladium (II) chloride-Triphenylphosphine, *ibid.*, **49**, 2245 (1976).
15. J. Osugi, Y. Takezaki, and A. Makita: Evaluation of P-V-A relations—The Most Probable Values of Compressibility Factor of Methane, *Rev. Phys. Chem. Japan*, **41**, 61 (1972).

II Free Radical Reactions

1. Y. Takezaki and S. Mori: Determination of Micro-Reactor Volume from the Transient Concentration Profile by Means of a Time-of-Flight Mass Spectrometer and the Application to the Rate Constant Measurement of Fast Reaction, $O+NO_2 \rightarrow NO+O_2$ and $N+NO \rightarrow N_2O$, *Bull. Inst. Chem. Res., Kyoto Univ.*, **45**, 388 (1967).
2. A. Ibuki and Y. Takezaki: Primary Processes in the Flash Photolysis of Dimethyl Carbonate Vapor, *ibid.*, **45**, 406 (1967).
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